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The crucial AFOSR support of this prestigious international meeting, the XIXth Conference on the Dynamics of Molecular Collisions, included participant support for invited speakers and other presenting authors. The AFOSR support, under award number F49620-03-1-0286, was $10,000, with a duration of 5/1/2003 - 12/31/2003. AFOSR has traditionally been generous in support of this meeting, as it draws a broad spectrum of the top researchers and young talent across several areas of direct interest to the AFOSR mission. The invited speakers included several with AFOSR funding, and the invited and contributing participants are drawn from both educational institutions and national laboratories.

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# Final Project Report: Participant Support for the XIXth Conference on the Dynamics of Molecular Collisions

Conference held July 13-18, 2003
Granlibakken Conference Center
Tahoe City, California

Chair of meeting and PI for AFOSR support: Laurie J. Butler

**Abstract**

The crucial AFOSR support of this prestigious international meeting, the XIXth Conference on the Dynamics of Molecular Collisions, included participant support for invited speakers and other presenting authors. The AFSOR support, under award number F49620-03-1-0286, was $10,000, with a duration of 5/1/2003 - 12/31/2003. AFOSR has traditionally been generous in support of this meeting, as it draws a broad spectrum of the top researchers and young talent across several areas of direct interest to the AFOSR mission. The invited speakers included several with AFOSR funding, and the invited and contributing participants are drawn from both educational institutions and national laboratories.

**Conference History and Scope**

The Dynamics of Molecular Collisions Conference draws participants interested in all aspects of molecular collision processes at the forefront of modern physical chemistry. Traditionally these have included experimental and theoretical studies of elastic, inelastic, and reactive encounters involving atoms, molecules, ions, clusters and surfaces, as well as half-collisions including photodissociation, photo-induced reactions and photodesorption. Speakers are chosen to represent the most exciting advances in both the core and multidisciplinary forefronts of the study of molecular collision processes, broadly defined. In recent years topics of central interest have included quantum dynamics of surface photoprocesses, coherent control in ultrafast chemical processes, radical photochemistry and reaction dynamics, and phase and amplitude control of molecular wavepackets. This meeting has had a distinguished history, beginning in 1965 as a Gordon Research Conference, and continuing independently when the number of participants grew to exceed the GRC limit. It is held now every two years.

The scientific program for the meeting in 2003 included the most exciting advances in these core areas and advances in new multidisciplinary studies of molecular collision processes. In 2003 the invited sessions covered topics ranging from bimolecular collision dynamics to interfacial dynamics in biological systems. In addition to the invited oral sessions and contributed poster sessions, the scientific program included a formal session consisting of five contributed talks selected from the submitted posters. The 2003 meeting, the nineteenth in the series, was organized and chaired by Prof. Laurie J. Butler, The University of Chicago, and vice-chaired by Dr. Al Wagner, Argonne National Laboratory. The responsibility of serving as sponsoring society, or agency, falls on the institutions of the chair and vice-chair for a given year.

Recent meetings in this series have been organized by James T. Muckerman (Brookhaven National Laboratory), James J. Valentini (Columbia University), George Schatz (Northwestern University), Daniel Neumark (University of California, Berkeley), Joel M. Bowman, (Emory University), and James Farrar (Rochester University). Although the meetings have been held in the United States, speakers and general attendance have always included a large component of participants from abroad. The meeting has thus always been international in scope.

**The Program in 2003 and Participation**

The scientific program at this meeting included both invited oral presentations, listed in Appendix A at the end of this report, and 115 contributed papers, also listed in Appendix A. The 2003 meeting drew 160 participants, listed in Appendix B (the 1999 and 2001 meetings in this series had 145 and 125 respectively.) The meeting retained the Gordon conference spirit with scientific discussion extending throughout the afternoon and long into the night in poster sessions, so stimulated cross-fertilization between senior scientists and students/postdocs. The participation of graduate students in this premiere meeting was supported in part by substantial funds from one of the host institutions; forty-seven graduate students participated in the meeting. As done for the first time in 2001 with great success, in 2003 five of the most significant contributed papers were selected for both poster and oral presentation. The invited speakers were chosen to represent the most exciting advances in both the core and multidisciplinary forefronts of molecular collision phenomena and were organized into scientific sessions given in Appendix A. We took care to span the field broadly defined, with speakers ranging from the long-established leaders, such as Nobel Prize awardee Yuan T. Lee, to the most exciting young scientists, such as Ka Yee Lee and Stuart Althorpe, doing pioneering work in both the core and multidisciplinary forefronts of the field.

**Impact on AFOSR Research**

The infusion of young talented scientists into the research areas critical to the AFOSR mission can be facilitated by a premiere meeting of this kind. While the chemistry and physics departments of many major research universities focus on establishing interdisciplinary areas such as nanoscience and biophysics, pioneering research in core areas such as chemical kinetics and dynamics and surface/materials chemistry and catalysis continue at both top universities and government laboratories. Such research is critical to the design and utilization of propellants and the development of materials robust to flight in the upper atmosphere. An important function of this conference is to bring together top Ph.D. students working in several areas of physical chemistry with the leading researchers at universities and national laboratories in these fields.

The invited speakers include Nobel Prize winner Yuan T. Lee, whose pioneering studies of O + hydrocarbon reactions in the 1980's and 1990's opened up the exact quantum mechanical prediction of elementary reactions key in oxygen atom reactions both in the gas phase and at surfaces; J rgen Troe, a major figure in chemical kinetics in the world for three decades; Bruce Kay and Bret Jackson, whose studies of chemical reactions at interfaces is key to understanding hot atom reactions at surfaces; Rainer Beck, whose work on the vibrationally mediated decomposition of methane at surfaces open up new avenues for controlling heterogeneous chemistry; as well as several top researchers who are funded by your program at AFOSR: Paul Dagdigian, Daniel Neumark, Millard Alexander, David Yarkony and Hanna Reisler. It is extremely important to bring Ph.D. students into contact with the breadth and excitement of such

research so that they consider positions in areas of research critical to the AFOSR upon graduation. To that end we have raised considerable money to support graduate student travel to the meeting; we hope AFOSR can provide partial travel support for domestic invited speakers, the premiere overseas invited speakers in this field for whom we do not have support, and a select few contributing scientists who are just initiating their research programs so do not yet have significant grant support.

**Meeting Format**

The meeting included nine half-day oral sessions and four poster sessions over five days. Each of the eight invited oral sessions has an overview talk (40 min. + 15 min discussion) and two or three research talks (21 total at 40 min. each + 15 min. for each discussion). The contributed oral session had five speakers selected from the most exciting contributed papers. Ample time was allotted to promote vigorous discussion; there were no parallel sessions. As this report is being submitted electronically, I will mail a copy of the program book for the meeting to our AFOSR program manager under separate cover.

**Dissemination of Proceedings**

The meeting was open to all applicants and was been publicized widely through the web (conference web site http://home.uchicago.edu/~ljb4/DMC2003.html) and various professional societies. The conference announcements were been distributed to a much wider mailing list than in previous years, with the kind cooperation of former organizers of major meetings in the US and in Europe. Although no publications or proceedings are produced in this meeting series, there are no restrictions on dissemination of results presented at the meeting. The book of abstracts for the meeting was distributed to all participants, with extras made publicly available, and posted on the web site.

**Summary of Funding**

Breakdown of Participant Support Costs supported by AFOSR funds:

| | |
|---|---|
| Support for domestic invited speakers (18 @ $300/speaker)<br>Dagdigian., Harding, Neumark, Sanov, Gray, Hase, Kay, Jackson, Alexander, Zwier, Reisler, Levy, K. Y. Lee, Schulten, Wagner, Truhlar, Bowman, Yarkony | $5,400 |
| Support for overseas invited speakers (5 @ $600/speaker) not covered by our PRFSE support<br>Halberstadt, Schinke, Meijer, Balint-Kurti, Orr-Ewing | $3,000 |
| Support for assistant professors w/o significant grant funding (4 @ $400/speaker) Wade, Shaffer, Mueller, Duffy | $1,600 |
| Total AFOSR support | $10,000 |

APPENDIX A

## Titles of Invited and Contributed Papers Presented Orally

### REACTIVE COLLISIONS I

**Paul Dagdigian**, *The Johns Hopkins University* [Overview]
Progress report on reactive collisions: Nonadiabatic effects, polyatomic reactions
**Larry Harding**, *Argonne National Laboratory*
Radical-Radical Reactions
**Kopin Liu**, IAMS, *Academica Sinica*
Imaging a polyatomic reaction: From product pair-correlation to reactive resonance
**Stuart Althorpe**, *University of Exeter*
Probing quantum reaction dynamics with plane wave packets

### INTERACTIONS AND DYNAMICS IN CLUSTERS

**Daniel Neumark**, *The University of California, Berkeley* [Overview]
Spectroscopy and dynamics in clusters spanning the molecular to nanodroplet size regimes
**Andrei Sanov**, *The University of Arizona, Tucson*
Photoelectron imaging of molecular cluster anions
**Stephen Gray**, *Argonne National Laboratory*
The role of reactant channel complexes in the $OH + CO \rightarrow H + CO_2$ reaction
**Nadine Halberstadt**, *Lab. Physique Quantique, IRSAMC*
$Ar\cdots I_2$: A model system for complex dynamics

### MOLECULE-SURFACE INTERACTIONS

**William Hase**, *Wayne State University* [Overview]
Dynamics of Energy Transfer and Chemical Reaction in Gas-Surface Collisions
**Bruce Kay**, *Pacific Northwest National Laboratory*
Molecular Beam Studies of Dynamics and Kinetics on Ice and Oxide Surfaces
**Rainer Beck**, *cole Polytechnique F d rale de Lausanne*
State resolved gas - surface reactivity of vibrationally excited methane prepared by pulsed laser radiation
**Bret Jackson**, *University of Massachusetts*
Eley-Rideal and Hot Atom Reactions on Metal and Graphite Surfaces

### PHOTODISSOCIATION AND ISOMERIZATION DYNAMICS

**Reinhard Schinke**, *Max Planck Institut, G ttingen* [Overview]
Dissociation of Molecules in Ground and Excited Electronic States
**Yuan T. Lee**, *Academica Sinica, Taiwan*
Isomerization and Dissociation of Aromatic Hydrocarbons
**Joel Bowman**, *Emory University*
Full-dimensionality quantum calculations of acetylene/vinylidene isomerization
**Hanna Reisler**, *University of Southern California*
Nonadiabatic interactions in the photochemistry of radicals and covalently bound dimers

### INELASTIC COLLISIONS

**Millard Alexander**, *University of Maryland* [Overview]
The long saga of the NO molecule in the investigation of inelastic scattering
**Timothy Zwier**, *Purdue University*
Laser probes of the potential energy landscapes and conformational isomerization dynamics of a series of flexible biomolecules
**Gerard Meijer**, *University of Nijmegen*
Deceleration and trapping of polar molecules

### NONADIABATIC REACTION DYNAMICS

**David Yarkony**, *The Johns Hopkins University* [Overview]
Beyond diabolical: Higher dimensional conical intersection
**Gabriel Balint-Kurti**, *University of Bristol*
Electronically Non-adiabatic Dynamics in Photodissociation and Reactive Scattering
**Donald Truhlar**, *The University of Minnesota, Minneapolis*
New Methods for the Theoretical Treatment of Electronically Nonadiabatic Reactions

### DYNAMICS AT BIOLOGICAL INTERFACES

**Donald Levy**, *The University of Chicago* [Overview]

Biological Molecules in the Gas Phase: Urocanic Acid, Coumaric Acid, and Anthranilic Acid

**Ka Yee Lee**, The University of Chicago
Collapse Mechanism in Lung Surfactant

**Klaus Schulten**, *Beckman Institute, Univ. of Illinois*
Elementary Molecular Processes in Vision

### REACTIVE COLLISIONS II

**Albert Wagner**, *Argonne National Laboratory* [Overview]
Progress report on reactive collisions: from dynamics to kinetics

**Piero Casavecchia**, *Universita di Perugia*
Crossed beam reactive scattering using *soft* electron-impact ionization for product detection: bridging the gap between dynamics and kinetics of polyatomic multi-channel reactions

**Andrew Orr-Ewing**, *University of Bristol*
The dynamics of reactions of chlorine atoms with organic molecules

**Juergen Troe** *Universitat Goettingen*
Capture processes in reaction kinetics

### SELECTED CONTRIBUTED PAPERS

**M.C. Bacchus-Montabonel**, *LaSIM, Lyon*
Non-Adiabatic Effects in the Photodissociation of Bromoacetyl Chloride

**Holger Vach**, *PICM cole Polytechnique, Palaiseau*
Internal State Excitation and Molecular Dissociation in the Surface Scattering of $(N_2)_n$ and $(O_2)_m$ Clusters

**K. G. McKendrick**, *Heriot-Watt University, Edinburgh*
Dynamics of Gas-Liquid Interfacial Reactions of Oxygen Atoms with Hydrocarbons

**Richard A. Loomis**, *Washington University, Saint Louis*
The dynamics of low-temperature collisions of He atoms with He···ICl in a supersonic expansion

**Eric T. Sevy**, *Brigham Young University*
Collisional Deactivation of Highly- Vibrationally Excited Aromatic Molecules by $CO_2$: Measuring and Predicting the Energy Transfer Probability Distribution Function

## Titles of Contributed Papers

**John R. Morris**, B. Scott Day, and Melinda Ferguson
The Role of Interfacial Hydrogen-Bonding in Gas-Surface Energy Exchange

**M.C. Bacchus-Montabonel**, B. Lasorne, N. Vreck, and M. Desouter-Lecomte
Non-Adiabatic Effects in the Photodissociation of Bromoacetyl Chloride

Hilary J. Crichton, Matthew L. Costen and **Kenneth G. McKendrick**
Collisional Energy Transfer in OH Using Polarisation Spectroscopy

**Lin Feng**, Xin Huang, Andrey V. Demyanenko, and Hanna Reisler
Spectroscopy and Photodissociation Dynamics of Hydroxymethyl Radicals ($CH_2OH$): The 3s and $3p_x$ Rydberg states

**Samantha Hawkins**, George Kumi, Sergey Malyk, Hanna Reisler, and Curt Wittig
FTIR study of $H_2O$ and $N_2O$ interactions on MgO(100)

**Xinchuan Huang**, Stuart Carter, Joel M. Bowman
Full-dimensional quantum calculations of protonated water and water dimer, $H_3O^+$ and $H_5O_2^+$

Alrik J. van den Brom, T. Peter Rakitzis, Theofanis N. Kitsopoulos, and **Maurice H. M. Janssen**
State-to-state photodynamics of OCS: The effects of the initial state and orientation on multiple surface and non-axial dynamics

**H. Kelso**, F. Ausfelder, D. A. Henderson, **K. G. McKendrick**
Direct Comparison of the Effects of Vibrational Excitation on the Reactions $O(^3P) + CH_4(v_3=2)$ and HCl(v=2)

**H. Kelso**, S. P. K. K hler, D. A. Henderson and **K. G. McKendrick**
Dynamics of Gas-Liquid Interfacial Reactions of Oxygen Atoms with Hydrocarbons

**Svetlana Malinovskaya**, Paul Berman, and Philip Bucksbaum
Coherent control of vibrational excitations by ultrafast pulse shaping

G. Richmond and **K. G. McKendrick**
State-to-State Collisional Energy Transfer in Electronically Excited CH Radicals

**Mark J. Perri**, Annalise L. Van Wyngarden , Kristie A. Boering , Jim Jr-Min Lin , and Yuan T. Lee
Dynamics of the $O(^1D) + CO$ oxygen isotope exchange reaction

**Ilana B. Pollack, Ian M. Konen**, Eunice X. J. Li, and Marsha I. Lester
Spectroscopic Characterization of HOONO and its Binding Energy via Infrared Action Spectroscopy

**T. Stoecklin**, A. Voronin, J.C.Rayez
Ultracold collision of $F_2$ with He: A comparative study with the He-$N_2$ collision

**Erin S. Whitney**, Alexander M. Zolot, David J. Nesbitt, and Anne B. McCoy
Quantum state-resolved reactive scattering of $F + C_2H_6 \rightarrow HF(v,J) + C_2H_5$

**Tiao Xie**, Dunyou Wang, and Joel M. Bowman
Quantum calculations of the $O(^3P)$+HCl reaction on the $^3A''$ and $^3A'$ surfaces

**Peng Zhang**, Keiji Morokuma, Nils Hansen, and Alec M. Wodtke
A Theoretical Study of the Potential Energy Surfaces of the Photodissociation of Cyclic $N_3$ Radical

**Dmitri Babikov**, Brian K. Kendrick, Robert B. Walker, and Russell T. Pack
Quantum Origin of Anomalous Isotope Effect in Ozone Formation

D.F. Coker, H. Dothe, **L. Chen**, N. Yu, and J.W. Duff
Excited State Potentials and Non-adibatic Couplings for $O_3^+$ Reactions

**Feng Chen** and Anne B. McCoy
Mixed quantum/classical approach to photodissociation of $H_2O$ (X 8594; A and Ar-$H_2O$ (X 8594; A)

**Eric Surber**, Richard Mabbs, and Andrei Sanov
Photoelectron Imaging Spectroscopy of Molecular and Cluster Anions

**Aaron B. Potter**, Vladimir Dribinski, Andrey V. Demyanenko, and Hanna Reisler
Exit channel dynamics in the UV photodissociation of the NO dimer: $(NO)_2 \rightarrow NO(A^2\Sigma^+) + NO(X^2\Pi)$

**Vladimir Dribinski**, Aaron B. Potter, and Hanna Reisler
Photoelectron imaging studies of the NO dimer

**Yuchuan Gong**, Vladimir I. Makarov, Brad R. Weiner
Photodissociation of Thiophosgene at 248 nm and 193 nm

**Rosendo Valero**, Drew A. McCormack, and Geert-Jan Kroes
Five- and full-dimensional wave packet calculations for the OH (v=0, j=0) + CO (v=0, j=0) $\rightarrow$ H + $CO_2$ reaction on several potential energy surfaces

**Bill Isa**, Kevin D. Gibson, and Steven. J. Sibener
Experimental and Simulation Study of Rare Gas Collision Dynamics with a 1-Decanthiol Monolayer

**Jens Riedel**, Cord Elsner, Attila Kuczmann,Falk Renth, Jie Wei, and FriedrichTemps
Dynamics of Hydrogen Elimination from Pyrrole and Indole Studied by Velocity Map Imaging

**Diego Troya** and George C. Schatz
Reaction Dynamics of Hyperthermal $O(^3P)$ Collisions with Hydrocarbon Self-Assembled Monolayers

**James K. Parker**, Walter A. Payne, Regina J. Cody, and Louis J. Stief
Kinetics of the H + $HC_3N$ Reaction from 200 to 298 K

Fernandez, Abel, **Viggiano, A.A.**; Williams, Skip; Troe, J rgen
The reaction of $O_2^+$ with $C_9H_{12}$ (n-propylbenzene) and $C_{10}H_{14}$ (n-butylbenzene) as a function of pressure and temperature: rate constants and collisional stabilization of the charge transfer product

**Leon F. Phillips**
Dynamics in the capillary-wave zone

**Alexandra Viel** and Wolfgang Eisfeld
Effect of higher order Jahn-Teller coupling on the nuclear dynamics

**Ronald S. Friedman**, Lorenz S. Cederbaum, Victor M. Ryaboy and Nimrod Moiseyev
Bound Molecular States Embedded in the Continuum and Arising from Conical Intersections

**Boris Nizamov** and Stephen R. Leone
Kinetics of $C_2H$ reactions with hydrocarbons and nitriles in the 104 K-298 K temperature range: Implications for the photochemistry of Titan

Weidong Zhou, Yan Yuan, and **Jingsong Zhang**
State-to-state Photodissociation Dynamics of OH Radical via the *A* state and Fine State Distributions of the $O(^3P_J)$ Product

**Jennifer L. Gardner** Steven M. Miller
Distribution of Rotational and Vibrational Energy in the HCO Product of the $O(^3P) + C_2H_4$ Reaction

**Jamie Matthews**, Melanie McWilliams, and Amitabha Sinha
Photodissociation of Vibrationally Excited Pernitric Acid: $HO_2NO_2(2v_{OH}) + 390$ nm

**Sally Chapman** and Kiryn Haslinger
Classical Trajectory Study of Energy Transfer in Collisions of hot Pyrazine with Diatomics

**Uros S. Tasic** and Charles S. Parmenter
Rate Constants for Vibrational Energy Transfer from Regions of the $S_1$ Vibrational Manifold of Para-difluorobenzene with High State Densities

R.G. Macdonald and **Yide Gao**
Time-resolved Absorption Studies of the Radical-atom Reaction

**Jose Lopez** and Anne B. McCoy
Transition State Dynamics Studies of $Ar_n$ ¥ IHI (n = 0, 2)

**Nils Hansen** and Alec M. Wodtke
Photodissociation Dynammics of $ClN_3$ : The Cl + $N_3$ Channel. Evidence for the Formation of the cyclic $N_3$ Isomer

**Ronald J. Duchovic**, Yuri L. Volobuev, Gillian C. Lynch, Ahren W. Jasperb, Donald G. Truhlar, Thomas C. Allison, Albert F. Wagner, Bruce C. Garrett, Jose C. Corchado, Joaquin Espinosa-Garcia
POTLIB 2001: A Potential Energy Surface Library for Chemical Systems

**Anne B. McCoy**, Mark S. Taylor, Felician Muntean and Carl Lineberger
Probing dissociation dynamics: Experimental and theoretical studies of the copper-water complex

**D. Stolyarov**, E. Polyakova and C. Wittig
Intramolecular Quantum Chaos in Doped Helium Nanodroplets

**C. Murray** , R.L. Toomes , A.J. Orr-Ewing and T.N. Kitsopoulos
State-resolved velocity map imaging of bimolecular reactions

Yide Gao and **R.G. Macdonald**
Time-resolved Absorption Studies of the Radical-Radical Reaction: NCO + $CH_3$

**James A. Gardner** and A. Lyle Broadfoot
Molecular Dynamics in the Ionosphere

**Holger Vach**, Nihed Chaabane, Quentin Brulin
Internal State Excitation and Molecular Dissociation in the Surface Scattering of $(N_2)_n$ and $(O_2)_m$ Clusters

**Girts Barinovs, Marc C. van Hemert**
Formation of Carbon-bearing molecules in the interstellar medium. The $CH^+$ and $CH_2^+$ cases.

**L. Valachovic**, R. B. Cohen
Dynamics of Insertion-type Reactions: $O(^1D) + CH_3OD$

**Ani Khachatrian**, Murthy S. Gudipati, Richard A. Copeland, and Marshall L. Ginter
Temperature Dependence of the Collisional Energy Transfer in $N_2(a^1\Pi_g$ and $a'^1\Sigma_u^-$, v=0,1)

**Xianghong Liu**, Richard L. Gross, and Arthur G. Suits
Crossed beam imaging study of Cl + alkane reactions

Sissi Li, Elizabeth Sklute, **Elisabeth Wade**, Bradley Parsons and David Chandler
Photodissociation of NO-Rare Gas Clusters

**M. E. Mandy**
Energy Transfer and Dissociation in Molecular Hydrogen: The Role of Internal Energy in the Collider

Richard Overstreet, Allan J. Shaffer, Chris Austin, and **James P. Shaffer**
A Stark Slower to Study Amide Chemistry

**T. Jayasekharan** and Charles S. Parmenter
A Puzzle in understanding the fluorescence spectrum of the pDFB-Ar complex

**Biswajit Maiti** and George C. Schatz
Theoretical studies of intersystem crossing effects in the nonadiabatic dynamics of bimolecular reactions

**R. C. Mowrey**, E. Pijper, G. J. Kroes, R. A. Olsen, and E. J. Baerends
Dissociative Adsorption of $H_2$ at the Pt(111) Top, Bridge, and FCC Surface Sites

Joshua P. Darr, David S. Boucher, Andrew C. Crowther, **Richard A. Loomis**, and Anne B. McCoy
Detailed characterization of the He + ICl(X,v"=0) and He + ICl(B,v') interactions and dissociation dynamics: A combined experimental and theoretical study

**Richard L. Gross**, Xianghong Liu, and Arthur G. Suits
$O(^3P)$ versus $O(^1D)$ Reaction Dynamics with n-Pentane: A Crossed-Beam Imaging Study

**Hans A. Bechtel**, Jon P. Camden, and Richard N. Zare
Investigating the reaction of Cl with vibrationally-excited $CH_4$: Is the effect of the symmetric ($\nu_1$) stretch different than the effect of the asymmetric ($\nu_3$) stretch?

**Shinnosuke Kawai**, Yo Fujimura and Okitsugu Kajimoto
Nascent Product State Distribution and Reaction Dynamics of $O(^1D)+N_2O$

Zhixin Tian and **Qihe Zhu**
A Simple High-resolution Photofragment Translational Spectrometer: Photodissociation of CF3I

Alexander M. Zolot, Erin S. Whitney, and David J. Nesbitt Quantum state-resolved reactive scattering of F + HCl ↔ HF(v,J) + Cl

P. Casavecchia, N. Balucani, G. Capozza, E. Segoloni
Crossed beam experiments versus exact quantum scattering calculations on *ab initio* potential energy surfaces for *abstraction* and *insertion* reactions: $Cl(^2P) + H_2$, $N(^2D) + H_2$, and $C(^1D) + H_2$

**P. Casavecchia**, N. Balucani, L. Cartechini, A. Bergeat, G. G. Volpi
Crossed beam reactive scattering of nitrogen atoms: the reaction dynamics of $N(^2D) + H_2O$ and $N(^2D) + CH_4$

**Sangwoon Yoon**, Robert J. Holiday, Edwin L. Sibert III and F. Fleming Crim
The relative reactivity of the symmetric stretch and the antisymmetric stretch of $CH_3D$ in the $CH_3D + Cl\ (^2P_{3/2})$ reaction

**Spiridoula Matsika** and David R. Yarkony
Beyond the Double Cone: a) Conical Intersections and Spin-Orbit Coupling in ClHCl, b) Three-State Conical Intersections in the Allyl Radical

H. Hippler, N. Krasteva, and **F. Striebel**
The thermal unimolecular decomposition of HCO

**David A. Dolson** and Farnaz Tabatabain
Electronic-to-Vibrational Energy Transfer from $Cl^*(^2P_{1/2})$ to $CF_4(\nu_3)$

**D. E. Szpunar**, M. L. Morton, Y. Liu, M. J. McCullagh, L. J. Butler, P. M. Regan and J. Shiu
Primary and secondary dissociation of allyl iodide and allyl-$d_2$ iodide excited at 193 nm

**Bradley F. Parsons** and David W. Chandler
Dissociation Dynamics of Charge Transfer Clusters

**Sean M. Casey** and Linhu Zhang
Chloroalkane interactions with room temperature silicon surfaces

**George C. McBane**
*Ab initio* thermal rate coefficients for rotational relaxation of CO: comparison with IR double resonance experiments

Paula Matei and **Brian Stewart**
Comparison of Diatomic Rotational Energy Transfer in Differnet Electroinic States

**Johanna L. Miller**, Maria J. Krisch, Melita L. Morton, Laurie J. Butler, Fei Qi and Jinian Shu
Dissociation Channels of the 1-Buten-2-yl Radical: An Experimental and *Ab Initio* Study

Jonathan J. Schroden, Ryan Z. Hinrichs, and **H. Floyd Davis**
Dynamics of C-C and C-H Bond Activation in Neutral Transition Metal-Hydrocarbon Reactions

**Konstantinos S. Kalogerakis**, Dusan A. Pejakovic , Richard A. Copeland, and Tom G. Slanger
Energy Transfer in $O_2(X^3\Sigma_g^-, v=1) + O(^3P)$ and $O_2(X^3\Sigma_g^-, v=2,3) + O_2$ Collisons

Christopher G. Elles, **M. Jocelyn Cox**, and F. Fleming Crim
Vibrational relaxation of $CH_3I$ in the gas phase and in solution

Sangwoon Yoon, **Robert J. Holiday**, and F. Fleming Crim
Control of bimolecular reactions: Bond-selected reaction of vibrationally excited $CH_3D$ with $Cl\ (^2P_{3/2})$

**David L. Osborn**
The Reactions HCCO + $O_2$ and HCCO + NO: Product State Distributions and Energy Transfer by Time-Resolved Fourier Transform Spectroscopy

**Jon P. Camden**, Hans A. Bechtel and Richard N. Zare
Experimental investigations of the scattering dynamics for the benchmark polyatomic reaction: $H+CD_4 \rightarrow CD_3+HD$

**Laurence A. Angel**, Moses K. Dogbevia, Katarzyna M. Rempala and **Kent M. Ervin**
Cross Sections and Product Velocity Distributions of the Hydrogen Atom Abstraction Reactions of $S^-$ with $H_2$, $CH_4$ and $C_2H_6$

**F. D. Colavecchia**, G. A. Parker, and R. T Pack
Accurate quantum reactive scattering calculations in spin-aligned $^7Li_3$systems

**Engelene t. H. Chrysostom**, James P. Schaffer, Albert Stolow, Anouk M. Rijs, Maurice H. M. Janssen, and Carl C. Hayden
Femtosecond Time-Resolved Photoelectron/Photoion Coincidence Imaging

Karl E. Jackson, Brian J. Hom, and **Eric T. Sevy**
Collisional Deactivation of Highly-Vibrationally Excited Aromatic Molecules by $CO_2$: Measuring and Predicting the Energy Transfer Probability Distribution Function.

**John M. Herbert** and John E. Harriman
Density matrix functional theory for strongly-correlated electronic states

**Yuri Georgievskii** and Stephen J. Klippenstein
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**F. Ausfelder**, A. E. Pomerantz and R. N. Zare
Collision energy dependence of the HD (v =2) rotational product state distribution of the H + $D_2$ reaction in the range of 1.3 to 1.9 eV

**Laura R. McCunn**, Maria J. Krisch, Kana Takematsu, Laurie J. Butler and Jinian Shu
Photodissociation of Propionyl Chloride at 193 and 248 nm

**Canay Ege**, Guohui Wu, Jarek Majewski, Kristian Kjaer, Sushil Satija, Ka Yee C. Lee
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**A. E. Pomerantz**, F. Ausfelder, and R. N. Zare
Potential applications of Doppler-free multiphoton ionization in dynamics experiments

**Liam M. Duffy**
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**Niel E. Sveum**, Jason C. Robinson, and Daniel M. Neumark
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**Mark F. Witinski**, Cheng Lin, Marivi Ortiz-Suarez, and H. Floyd Davis
Dynamics Studies Using Rydberg Atom Time-of-Flight Spectroscopy

**Xiao-Gang Wang** and Tucker Carrington Jr.
Vibrations of methane : a numerically exact solution of a nine-dimensional Schroedinger equation

**M. J. Krisch**, J. L. Miller , L. J. Butler, H. Su, R. Bersohn, and J. Shu
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**Dusan A. Pejakovic**, Philip C. Cosby, Richard A. Copeland, and Tom G. Slanger
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**Yi Zhao**, Takeshi Yamamoto, and William H. Miller
Quantum Instanton Approximation for Thermal Rate Constants of H + $CH_4 \rightarrow CH_3 + H_2$

**M. Ceotto** , W. H. Miller , Y. Zhao , S. Yang
Quantum Instanton Approximation for Thermal Rate Constants of Chemical Reactions

**Yimin Lee** and William H. Miller
A Semiclassical Time-Dependent Wavepacket Approach for the Calculation of Reaction Probability

**F. Paesani**, R. Zillich and K.B. Whaley
OCS in small para-hydrogen clusters: energetics, structures and superfluidity<.a>

**S. Yang** and W. H. Miller
Some new developments in the application of Quantum Instanton model to rate constant calculation

**M. Shane Bowen**, Daniel C. Luhrs, and Robert E. Continettti
Stable and Dissociative Photodetachment Studies of $C_3H_5O^-$ and $C_3H_4OH^-$

**Christopher M. Laperle**, Elad Harel, Jennifer Mann and Robert E. Continettti
Charge Exchange Dynamics of Molecular and Cluster Cations

**Zhou Lu** and Robert E. Continettti
Dissociative Photodetachment Study of the Acetate Anion

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Femtosecond Valence and Core Photoelectron Molecular Dynamics

**Dunyou Wang**, Winifred M. Huo, Christopher E. Dateo, David W. Schwenke, James R. Stallcop
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**B. Lasorne**, M. Desouter-Lecomte, D. Lauvergnat, and G. Dive
Quantum dynamics in reduced dimensionality

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Non-Adiabatic Dynamics of B + $H_2$

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**Robert E. Zillich** and K. Birgitta Whaley
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**David W. Chandler**
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**S. C. Althorpe**
Time-dependent quantum description of Ar + NO: does the scattered NO rotate clockwise or anticlockwise, and why?

Levi J. Collier and **Julie A. Mueller**
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Yuval Ganot, Amir Golan, Salman Rosenwaks and **Ilana Bar**
Non-adiabatic dissociation of rovibrationally excited acetylene

B. Ruscic, **M. L. Morton**, R. E. Pinzon, B. Wang, A. F. Wagner Photoionization Mass Spectroscopy as a Means to Produce Reliable Thermochemical Values for Input into the Active Thermodynamics Tables"

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